2-(1-Hydroxy-1-methylethyl-2-methyl-1,3-dioxane

39239-96-8 | DTXSID80192497

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 37.9 °C

Global applicability domain: Inside

Local applicability domain index: 4.17e-01

Confidence level: 5.40e-01

Nearest Neighbors from the Training Set

Image not found
Ethyl mandelate
Measured: 35.0
Predicted: 48.7

Image not found
Diacetone alcohol
Measured: -44.0
Predicted: -27.9

Image not found
Methylephedrine
Measured: 87.5
Predicted: 90.6

Image not found
Phenol, 3,5-dimethoxy-
Measured: 37.0
Predicted: 55.4

Image not found
Xanthoxyline
Measured: 82.0
Predicted: 72.7